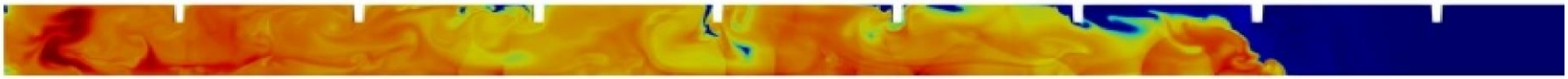
Numerical Investigation of the Effect of Obstacle Shape on DDT in a Hydrogen-Air Mixture



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Outline

- Introduction
- Motivation and Goals
- Background
- Simulation Approach
- Results and Discussion
  - Several cases with different obstacle shapes
- Conclusions
- Questions

Introduction

- UC Davis
  - Aerospace and Mechanical Engineering
  - Worked with Professor Robinson
- Stanford University
  - Aeronautics and Astronautics Department
  - PhD Candidate working with Professor Cantwell
  - Computational combustion research
- NASA Ames Research Center
  - Pathways intern
  - Engineering Risk Assessment Team
  - Advanced Supercomputing Division

Motivation

- Many situations where understanding the risk to human safety in the event of large, explosive failures is important
- Ignition energy for hydrogen is very low
  - Weak ignition source can result in transition to detonation
- We care about risk to crew safety if an uncontained failure occurs in a rocket engine bay

https://en.wikipedia.org/wiki/Cygnus_CRS_Orb-3

Goals

- Want to be able to reliably determine:
  - Flame speed and location
  - Overpressures
  - Potential for DDT
- Look to add better chemistry models and unique geometries that focus on specific aspects of the flow to better understand DDT
- Results will guide future risk assessments

Background

- **Deflagration**: Combustion that propagates through a gas at subsonic speeds, driven by heat transfer
- **Detonation**: Combustion where the flame front is supersonic, shock wave right in front of it
- **DDT**: Deflagration to Detonation Transition
- **Direct Initiation**: Large enough external energy to directly ignite detonation
- **Indirect Initiation**: Weak energy source (mJ), subsonic wave ignited, accelerates to detonation (DDT)

Approach

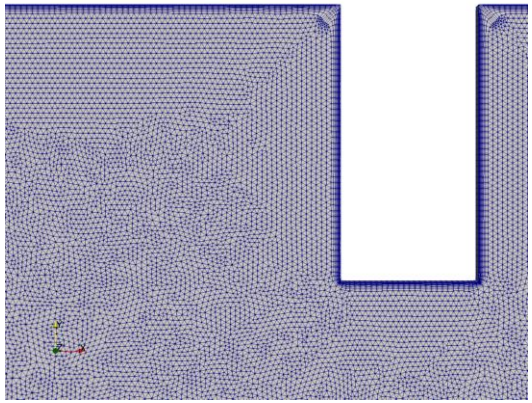
Code

- Computational fluid dynamics code Loci-Chem
- Originally developed at Mississippi State
- Density-based, finite-volume, unstructured solver with second order accuracy in time and space
- Capable of solving the Navier-Stokes equations for three dimensional, non-equilibrium, viscous, turbulent, and chemically reacting flows

Approach

Mesh

- Mesh parameters consistent between all geometries
- Generated unstructured, isotropic grids with an advancing front algorithm
- Axisymmetric geometries allowed for 2D mesh
- Mesh size = 125 μm



Approach

Chemistry

- Stoichiometric premixed hydrogen-air
- 7 species, 8 reaction model
  - Many studies just use 1 step model since chemistry is computationally expensive
- Reaction rates described by an Arrhenius model

Turbulence

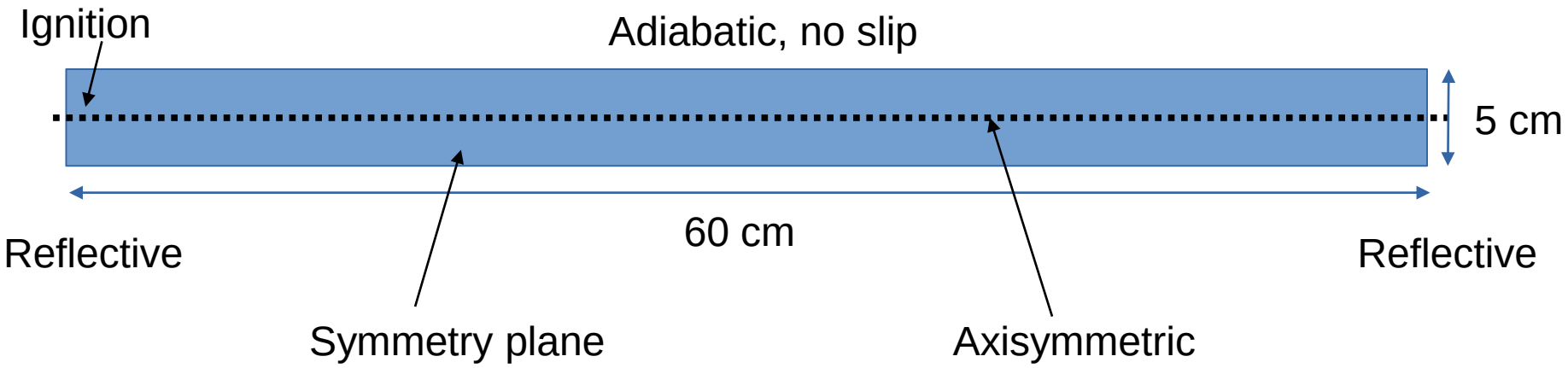
- Mentor's Baseline Model – works well for high speed flows
- Barth flux limiter – stable at high pressures

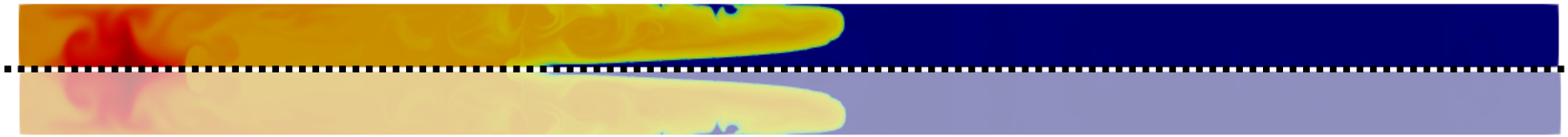
Results and Discussion

- Interested in flame propagation in a confined space and the potential for flame acceleration and DDT
- Obstacles shorten distance and time to DDT
- Considered tubes with different obstacle shapes
  - No obstacles
  - Rectangular obstacles
  - Curved obstacles
  - Forward rectangular, Aft curved obstacles
  - Forward curved, Aft rectangular obstacles

Unobstructed Tube

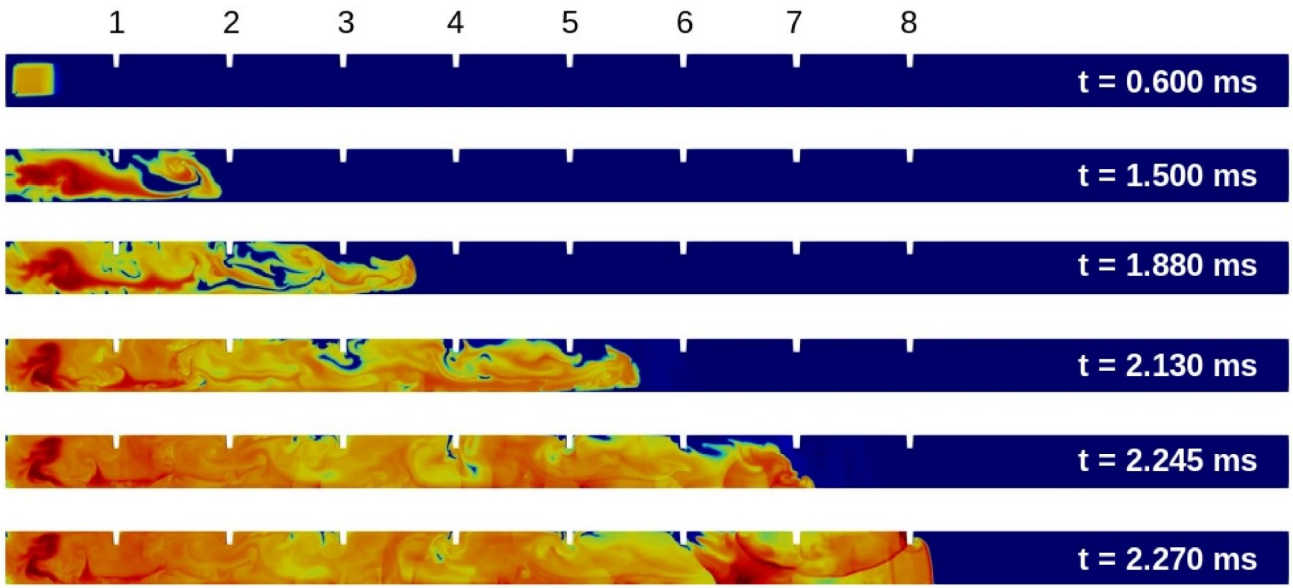
- Baseline Case
- Flow did not accelerate or transition to detonation
- Developed a distorted tulip flame





Rectangular Obstacles

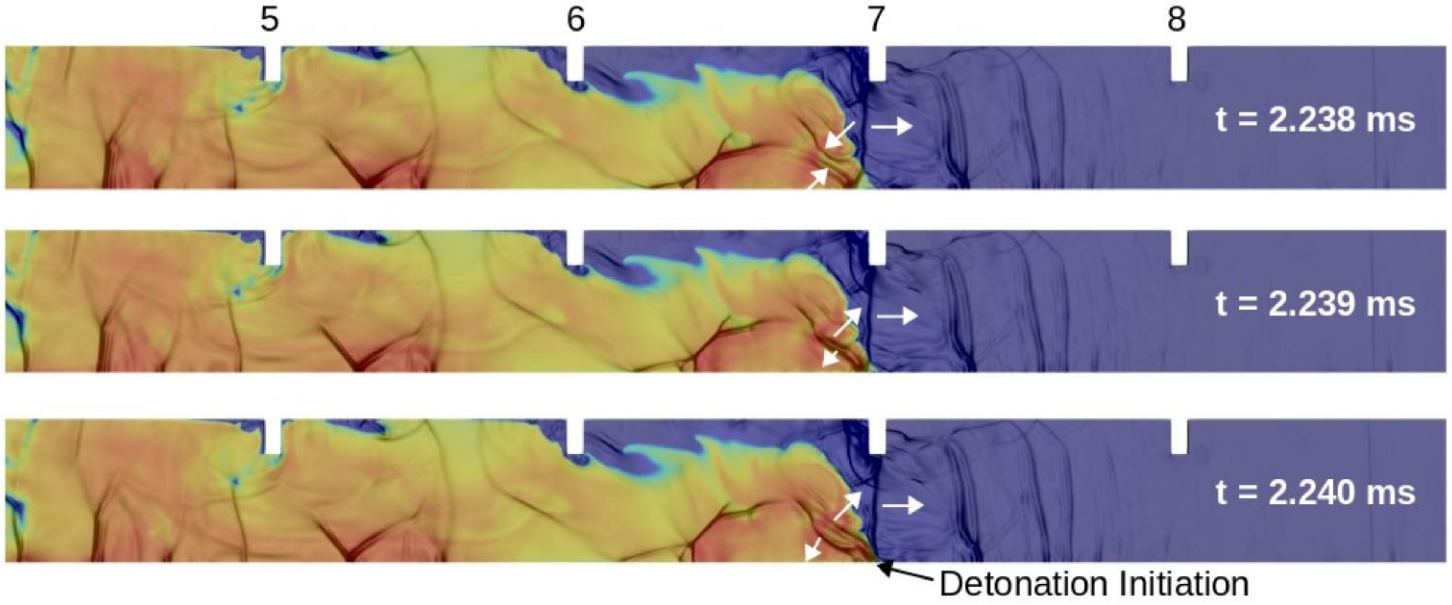
- Significant literature for rectangular obstacles
- 8 evenly spaced obstacles, 1 diameter apart
- Blockage ratio 0.43
- Flow detonates at obstacle 7



Rectangular Obstacles

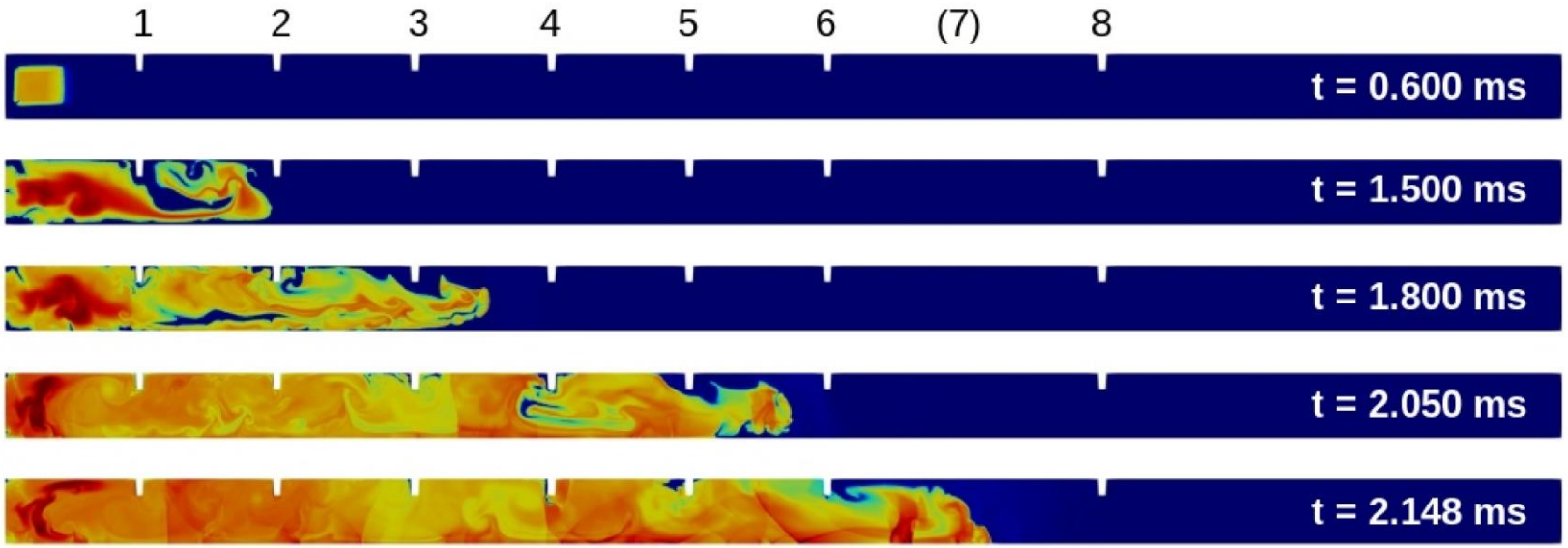
Rectangular Obstacles

- Pressure waves generate from hot expanding gas, reflect off walls and obstacles
- Detonation initiation occurs where strong pressure waves coalesce in unburned fuel at flame front



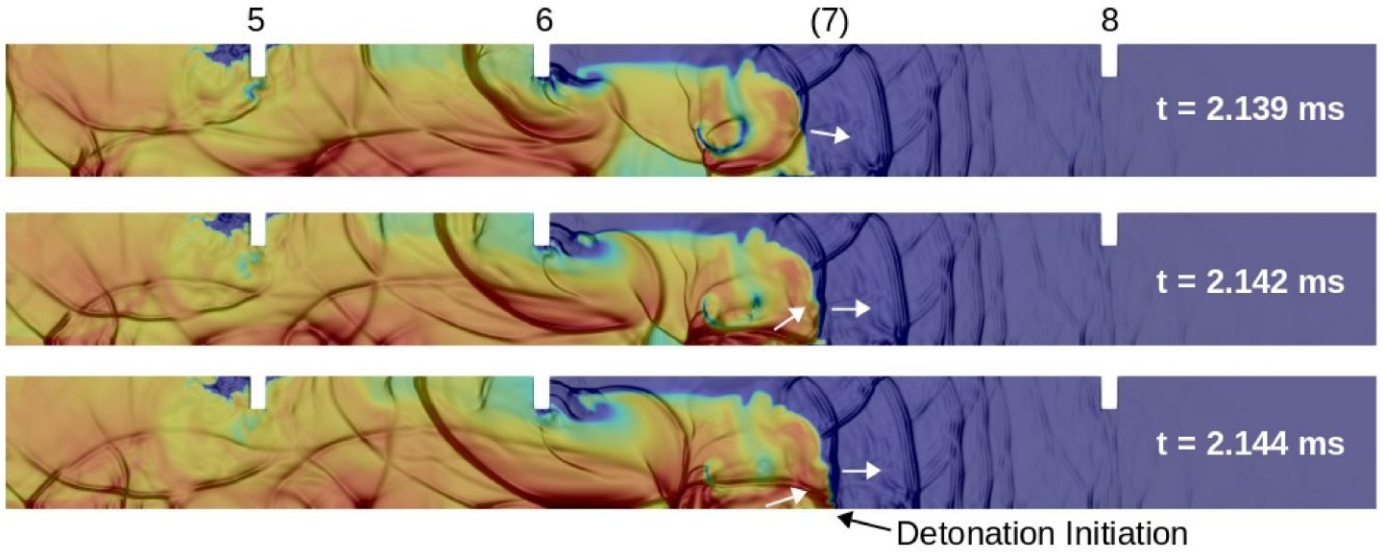
Obstacle 7 Eliminated

- Investigate the sensitivity of specific obstacle placement
- Eliminate obstacle at point of detonation
- Flow detonates at same location

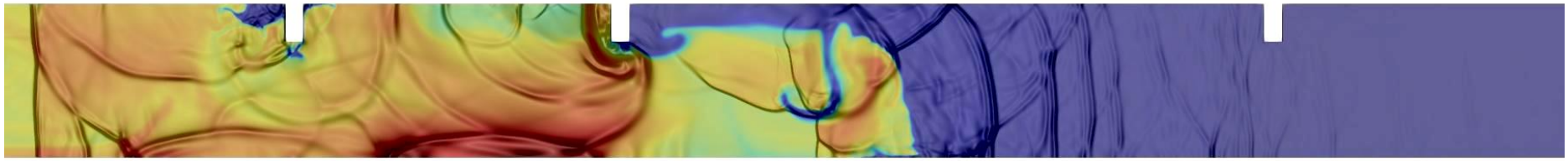


Obstacle 7 Eliminated

- Pressure waves near the wall did not coalesce, otherwise similar to previous case
- DDT is not that sensitive to exact obstacle placement or reflections off a specific obstacle
- Interesting result since several studies suggest pressure reflections at obstacles are crucial

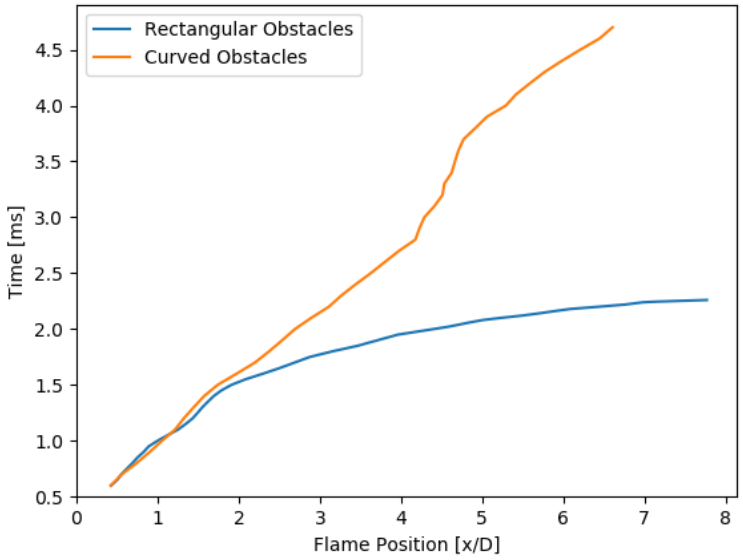


Obstacle 7 Eliminated



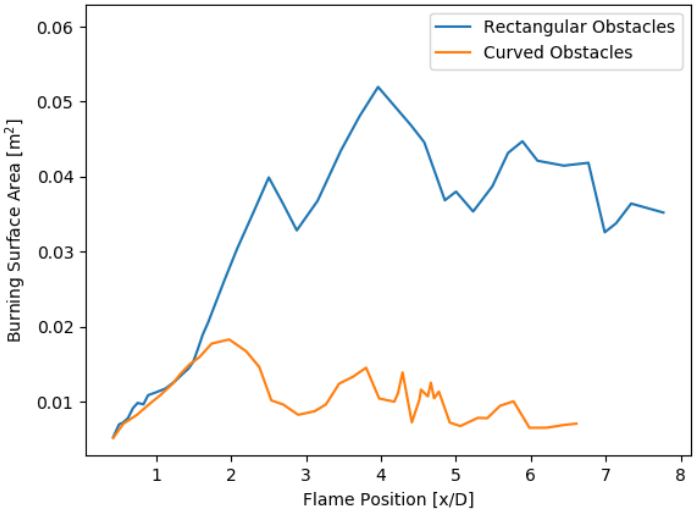
Curved Obstacles

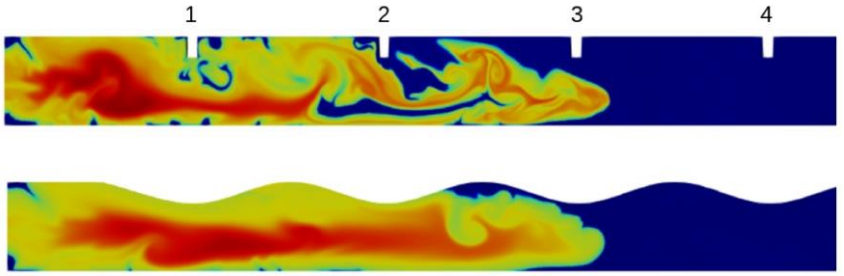
- One obstacle didn't change much, bigger change here
- Remove all forward corner reflections, reduce aft separation zone
- Keep blockage ratio the same
- Flame did not accelerate or detonate – looks more like unobstructed case



Curved Obstacles

- Why did curved obstacles not accelerate?
  - Turbulence/mixing
  - Burning surface area
- Rectangular obstacles had smaller scale turbulence
- More mixing, more flame burning surface area
- More burning area, more energy addition and the flow accelerates



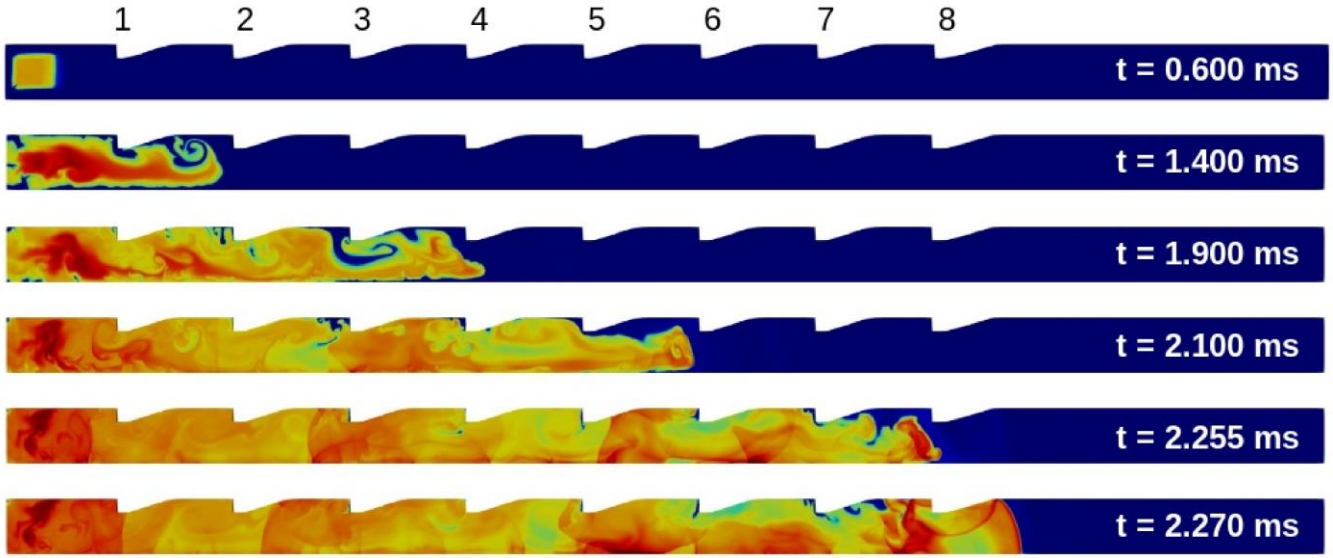


Forward Rectangular, Aft Curved

- Pressure waves and acceleration have proved important, now look at them separately
- Same spacing and blockage ratio
- Allowed forward corner reflections while reducing aft flow separation and recirculation zones
- Goal is to look at pressure wave reflections off obstacles while reducing mixing aft of obstacles

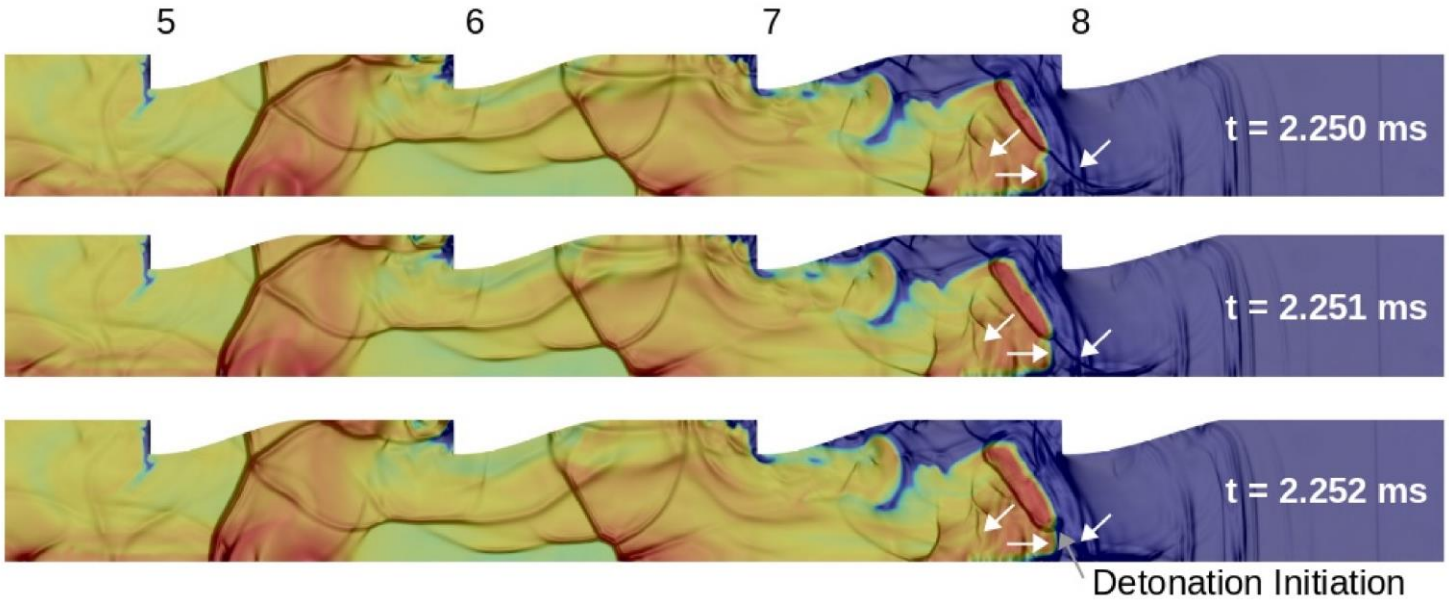
Forward Rectangular, Aft Curved

- Similar flow characteristics to rectangular obstacles
- Visible breaking up of the flow despite removing aft bluff body, separates off the forward part of the obstacle
- Detonated one obstacle later, not on center line



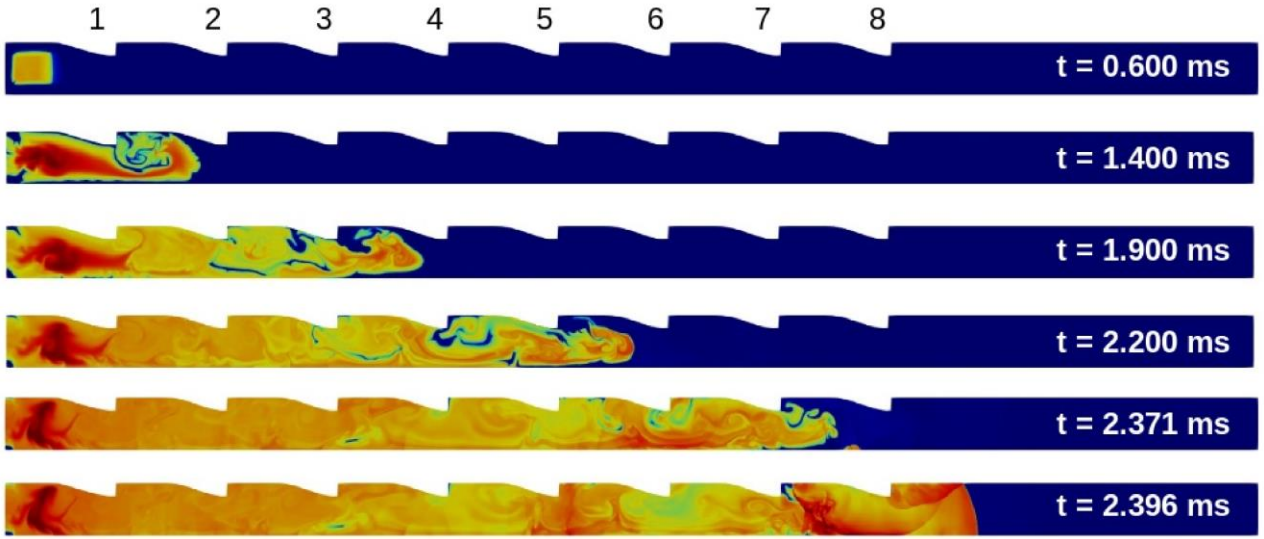
Forward Rectangular, Aft Curved

- Detonation mechanism relatively insensitive to exact obstacle placement and shape
- Just need acceleration and pressure wave reflections off something



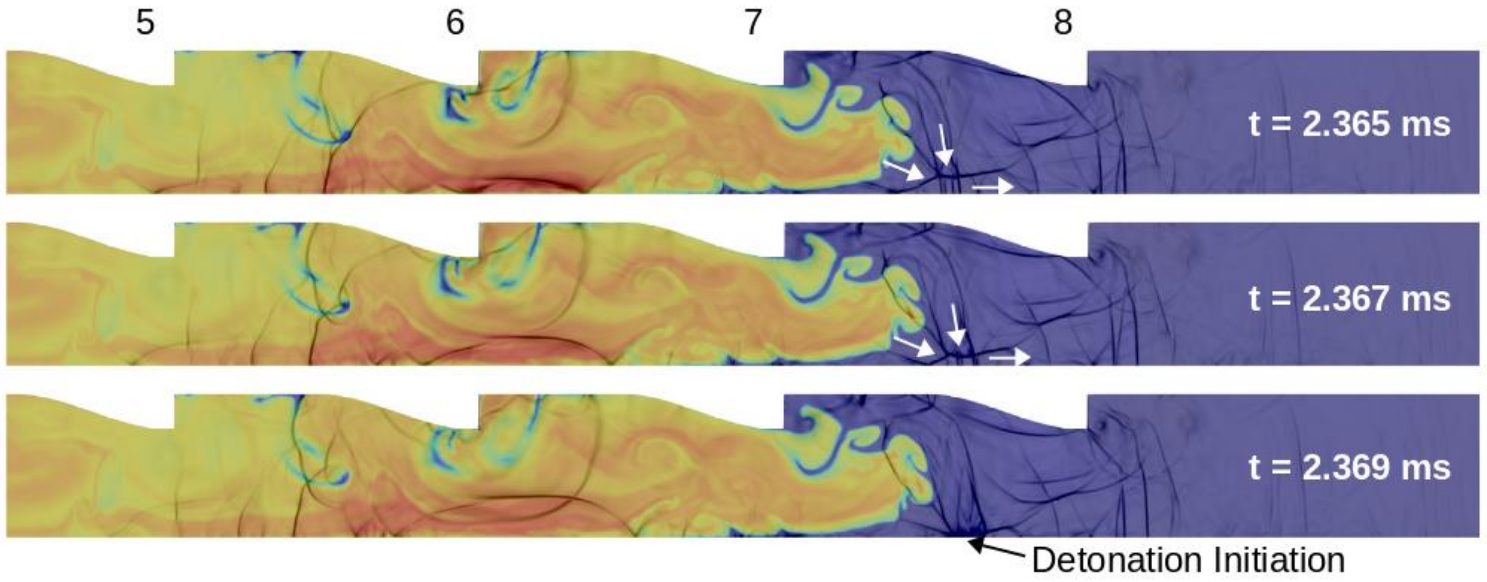
Forward Curved, Aft Rectangular

- Reversed the obstacles
- Allowed bluff body separation to increase mixing without forward corner pressure reflections
- Similar flow characteristics to rectangular obstacles
- Detonated ahead of the flame

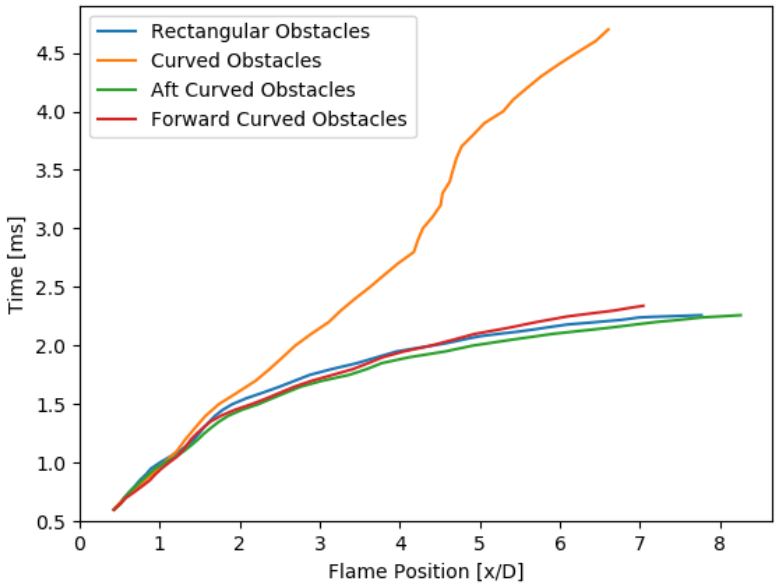


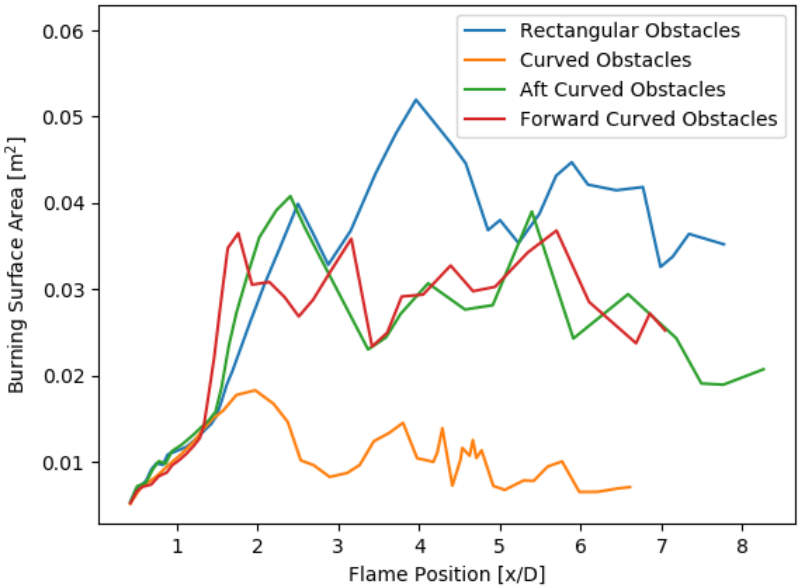
Forward Curved, Aft Rectangular

- Strong pressure wave reflections are still able to form despite removing forward corner reflections by curving the obstacle
- Pressure waves and reflections coalesce ahead of the flame front



Comparisons





- Mixed cases had smaller scale turbulence, more burning surface area, and accelerated flow
- Similar burning surface area for the mixed cases, similar energy addition
  - Difference in detonation is due to geometry and where pressure waves can coalesce

Conclusions

- Two main flow conditions must be met for DDT
  - Near-field confinement that results in reflections of strong pressure waves, waves must interact in unburned fuel
  - Flow must have sufficient energy resulting in acceleration – flow constriction is not sufficient, obstacles must encourage small scale mixing to increase burning surface area which accelerates the flow
- Geometry must set up pressure wave reflections and mixing, but a specific obstacle placement or geometry is not required for DDT

Future Work

- Continue eliminating obstacles to determine how many are actually needed
- Look at smooth wall case in more detail
- Consider ways to detonate faster
  - More energy
  - Different ignition configuration
- Move towards applications

Questions?